Hair Today

Product developers in the cosmetics industry can put simulation to use in performing hierarchical analyses of hair care product performance.

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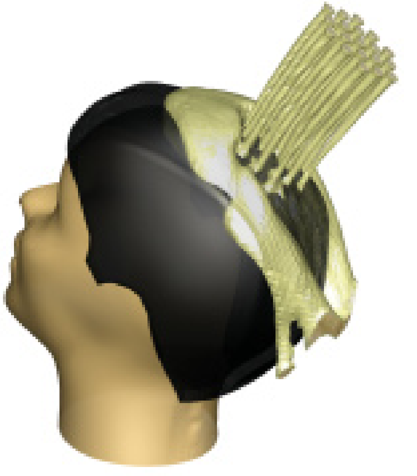


Simulation of water flow rinsing process using head-scale modeling

In the consumer-driven world of cosmetics, consumer experience and expectations are anything but an exact science. Qualitative performance testing, to gather information such as “Does this product increase hair’s shine?” or “Does this product spread through the hair well?” usually is achieved through subjective testing. As an alternative to such testing, product developers and researchers can use computational fluid dynamics (CFD) coupled with appropriate surface science and emulsion decomposition mechanisms for virtual testing of hair care products.

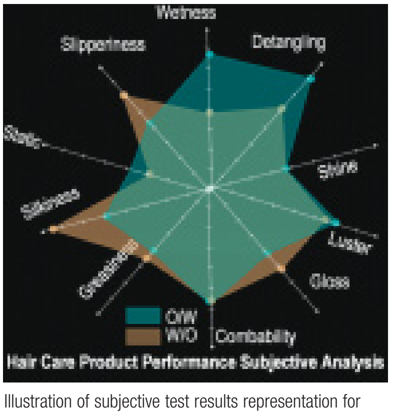
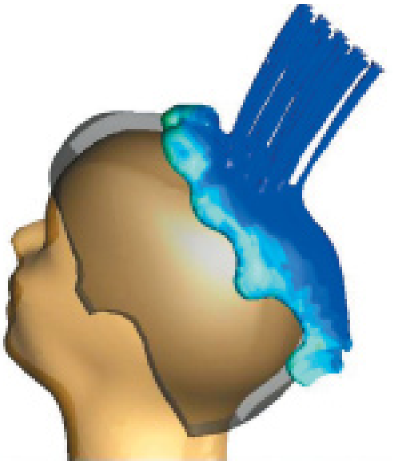


Illustration of subjective test results representation for two hair care systems

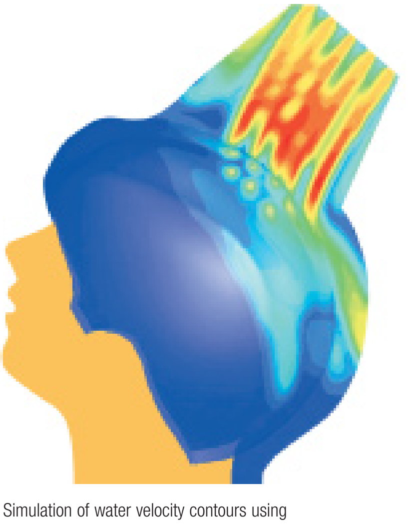
In order to mimic the subjective test procedure, a standard (baseline) hair with the standard (baseline) product can be simulated at the outset to establish quantitative correlations between subjective characteristics and chemical or fluid properties. Examples include the measurement of tackiness associated with surface tension, greasiness with viscosity and resulting glossiness with optical reflectance. As simulation progresses and correlations are developed, product developers also need to understand how and what to model on various scales.

Consistency in simulation is only as reliable as the details of physics and chemistry in the models. Within a predefined scope, simulation provides controlled test conditions. For example, a simulation-driven test procedure could be set up to begin with a known test subject, possibly developed within a “hair library” in the simulation software, of specified morphology, age, pore size, moisture absorption properties, temperature, and grease in and on the hair. The researcher then could define the environment around the test material (a sample hair assembly or tress) and apply the product making various assumptions, such as the choice to define application such that it yields approximately a uniform layer on the head. More detailed options include an applicator or a fingertip for studying the spreading and coating.

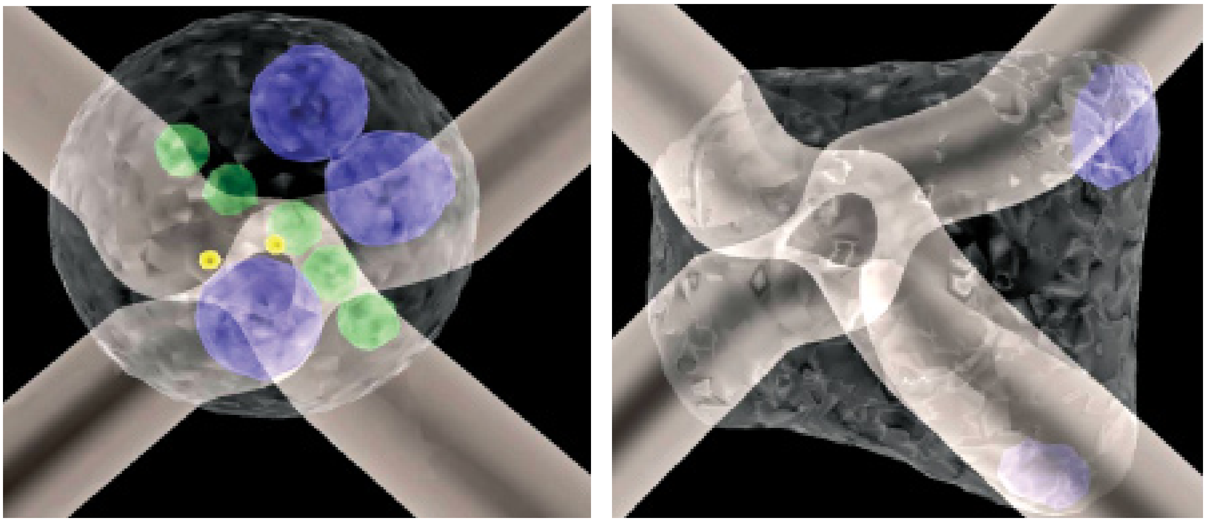


Simulation of shampoo concentration contours using head-scale modeling

Varying size and scope of the CFD model can provide insight for behaviors that are best observed on various scales. Product application and spreading can be accurately modeled on a relatively large “head-scale,” while functions such as glosser binding, which actually occur at the hair surfaces, are best modeled at a much smaller “hair-scale.” An effective



Simulation of water velocity contours using head-scale modeling



Spread of a complex oil droplet over a pair of cross-hairs: on the left, initial state in which ingredients suspended in the product's emulsion are represented as sub-droplets in the larger drop; on the right, the state after spreading has occurred

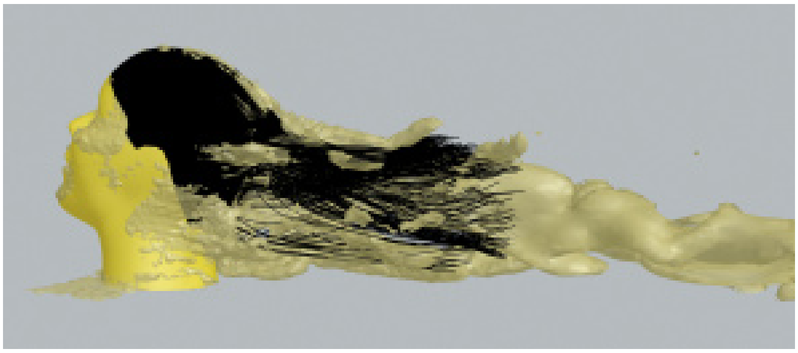
overall modeling approach involves coupling external flow with micro-phenomena near the hair surface. With this method, based on the large-scale flow conditions, the model is used to extract useful hydrodynamics data down to microscopic fluid volumes near a single hair and locally evaluate performance of various agents. This would enable gathering detailed information about the effectiveness of factors such as grease removal rate or product decomposition, which is relatively difficult, if not impossible, to consistently observe through tress-based tests.

Hair care products usually are packaged as emulsions, multi-liquid dispersions with suspended ingredients that don't segregate while stored. They are designed to dilute and break down when applied to the head with either fingers or a stream of shower. Variations in properties such as density, rheology, surface energy, chemical potential, temperature and phase-equilibrium of different immiscible and dissolving ingredients pose the design challenges to product developers. To understand the product breakdown process that occurs during application, a hair-scale simulation is required.

To examine the emulsion decomposition process, a complex, multiphase simulation is performed. A drop of the specified product is deposited at a location at which two hairs cross. The drop being modeled is about three times the hair diameter and includes suspended sub-droplets intended to represent the elemental ingredients in the emulsion. The simulation demonstrates the capillary effects of the cross-hair assembly and provides the product designer with information on the state of decomposition and spread of the product that will occur on such cross-hair configurations. Due to a variety of governing physics and the dissolution kinetics, pretreated hairs as well as conditioner ingredients greatly affect surface forces on the product drop that is being decomposed and spread.

The embedded constituents can be further defined to have their own specific material properties. For example, they could be defined as wettable, which means they stick to the hair, thereby serving as active deposition sites for various ingredients. In a case involving ingredients that are responsible for "hold" qualities, the sub-droplets could be defined as polymers that will undergo glass transition, leading to a firmer film at room temperature. This film structure will provide added elastic strength for the hair strand and evolve as a hold quality. One complexity for these films is that they will neither be exactly homogeneous in content nor have isotropic properties for factors such as elasticity, smoothness or thickness.

It is possible to set up a range of simulations for different starting compositions, sizes, temperatures and environmental dilutions and then to observe the final state for each distinct model. Although each simulation will predict a single resulting state, as though the product is in fact homogeneous and isotropic, a heuristic compilation of multiple simulations can together provide a more realistic statistical representation and characterization of the relative performances of various formulations. ■



Dynamic simulation of long hairs in a liquid stream